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Towards a Topological Basis for the Properties of Compressed Inorganic Glasses

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Temperature-dependent constraint theory has successfully been applied to explain and quantitatively predict the composition dependence of macroscopic glass properties, most notably equilibrium liquid viscosity for chalcogenide, borate, borosilicate, phosphate, and borophosphate glass-forming systems. According to this theory, the topological constraints are counted as a function of both composition and temperature, since any given constraint will be broken at a sufficiently high temperature. However, glass structure, topology, and properties also vary as a function of pressure, and it is thus of interest to develop a tool for predicting the changes in macroscopic properties upon compression. Indeed molecular dynamics simulations have shown that the rigidity of topological constraints depends on pressure in addition to temperature, i.e., it should in principle be possible to develop pressure-dependent constraint theory with predictive capability. Here, we present our recent findings with respect to establishing a topological basis for selected properties of compressed oxide glasses, which in turn could lead to the development of a predictive model for designing compressed glasses with optimized properties.